



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 12, 2024 – 04:16 AM EST

PDB ID : 3H4P
Title : Proteasome 20S core particle from Methanocaldococcus jannaschii
Authors : Jeffrey, P.D.; Zhang, F.; Hu, M.; Tian, G.; Zhang, P.; Finley, D.; Shi, Y.
Deposited on : 2009-04-20
Resolution : 4.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

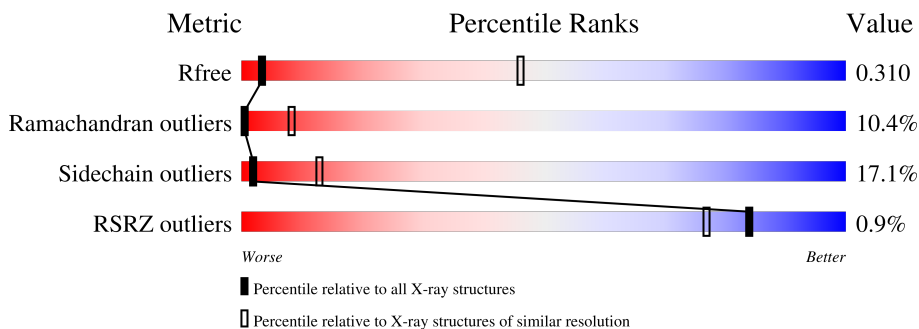
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1193 (4.50-3.70)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	264	 2% 71% 16% • 12%
1	B	264	 % 69% 17% • 12%
1	C	264	 % 70% 16% • 12%
1	D	264	 % 69% 17% • 12%
1	E	264	 3% 68% 18% • 12%
1	F	264	 2% 68% 18% • 12%
1	G	264	 % 69% 17% • 12%

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Mol	Chain	Length	Quality of chain
1	H	264	66% 20% • 12%
1	I	264	68% 18% • 12%
1	J	264	70% 16% • 12%
1	K	264	69% 18% • 12%
1	L	264	67% 19% • 12%
1	M	264	69% 18% • 12%
1	N	264	70% 17% • 12%
2	a	219	73% 17% • 8%
2	b	219	69% 20% • 8%
2	c	219	74% 14% • 8%
2	d	219	68% 22% • 8%
2	e	219	68% 22% • 8%
2	f	219	70% 18% • 8%
2	g	219	69% 19% • 8%
2	h	219	68% 22% • 8%
2	i	219	68% 21% • 8%
2	j	219	70% 20% • 8%
2	k	219	70% 19% • 8%
2	l	219	69% 19% • 8%
2	m	219	68% 21% • 8%
2	n	219	73% 16% • 8%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 46648 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	232	1813	1150	312	346	5	0	0	0
1	B	232	1813	1150	312	346	5	0	0	0
1	C	232	1813	1150	312	346	5	0	0	0
1	D	232	1813	1150	312	346	5	0	0	0
1	E	232	1813	1150	312	346	5	0	0	0
1	F	232	1813	1150	312	346	5	0	0	0
1	G	232	1813	1150	312	346	5	0	0	0
1	H	232	1813	1150	312	346	5	0	0	0
1	I	232	1813	1150	312	346	5	0	0	0
1	J	232	1813	1150	312	346	5	0	0	0
1	K	232	1813	1150	312	346	5	0	0	0
1	L	232	1813	1150	312	346	5	0	0	0
1	M	232	1813	1150	312	346	5	0	0	0
1	N	232	1813	1150	312	346	5	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q60177

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q60177
A	0	HIS	-	expression tag	UNP Q60177
B	-2	GLY	-	expression tag	UNP Q60177
B	-1	SER	-	expression tag	UNP Q60177
B	0	HIS	-	expression tag	UNP Q60177
C	-2	GLY	-	expression tag	UNP Q60177
C	-1	SER	-	expression tag	UNP Q60177
C	0	HIS	-	expression tag	UNP Q60177
D	-2	GLY	-	expression tag	UNP Q60177
D	-1	SER	-	expression tag	UNP Q60177
D	0	HIS	-	expression tag	UNP Q60177
E	-2	GLY	-	expression tag	UNP Q60177
E	-1	SER	-	expression tag	UNP Q60177
E	0	HIS	-	expression tag	UNP Q60177
F	-2	GLY	-	expression tag	UNP Q60177
F	-1	SER	-	expression tag	UNP Q60177
F	0	HIS	-	expression tag	UNP Q60177
G	-2	GLY	-	expression tag	UNP Q60177
G	-1	SER	-	expression tag	UNP Q60177
G	0	HIS	-	expression tag	UNP Q60177
H	-2	GLY	-	expression tag	UNP Q60177
H	-1	SER	-	expression tag	UNP Q60177
H	0	HIS	-	expression tag	UNP Q60177
I	-2	GLY	-	expression tag	UNP Q60177
I	-1	SER	-	expression tag	UNP Q60177
I	0	HIS	-	expression tag	UNP Q60177
J	-2	GLY	-	expression tag	UNP Q60177
J	-1	SER	-	expression tag	UNP Q60177
J	0	HIS	-	expression tag	UNP Q60177
K	-2	GLY	-	expression tag	UNP Q60177
K	-1	SER	-	expression tag	UNP Q60177
K	0	HIS	-	expression tag	UNP Q60177
L	-2	GLY	-	expression tag	UNP Q60177
L	-1	SER	-	expression tag	UNP Q60177
L	0	HIS	-	expression tag	UNP Q60177
M	-2	GLY	-	expression tag	UNP Q60177
M	-1	SER	-	expression tag	UNP Q60177
M	0	HIS	-	expression tag	UNP Q60177
N	-2	GLY	-	expression tag	UNP Q60177
N	-1	SER	-	expression tag	UNP Q60177
N	0	HIS	-	expression tag	UNP Q60177

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	b	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	c	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	d	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	e	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	f	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	g	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	h	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	i	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	j	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	k	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	l	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	m	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			
2	n	202	Total	C	N	O	S	0	0	0
			1519	964	248	298	9			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	6	MET	-	expression tag	UNP Q58634
b	6	MET	-	expression tag	UNP Q58634
c	6	MET	-	expression tag	UNP Q58634
d	6	MET	-	expression tag	UNP Q58634
e	6	MET	-	expression tag	UNP Q58634
f	6	MET	-	expression tag	UNP Q58634
g	6	MET	-	expression tag	UNP Q58634
h	6	MET	-	expression tag	UNP Q58634
i	6	MET	-	expression tag	UNP Q58634
j	6	MET	-	expression tag	UNP Q58634
k	6	MET	-	expression tag	UNP Q58634
l	6	MET	-	expression tag	UNP Q58634

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Chain	Residue	Modelled	Actual	Comment	Reference
m	6	MET	-	expression tag	UNP Q58634
n	6	MET	-	expression tag	UNP Q58634

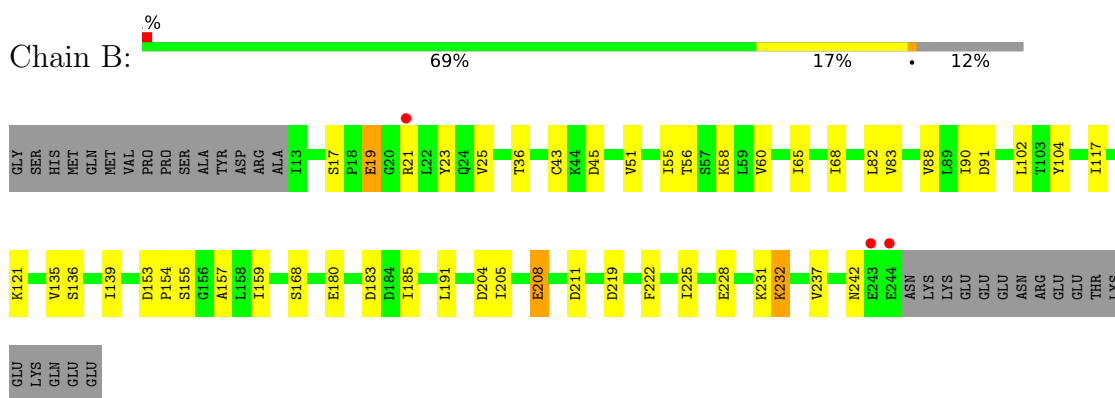
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

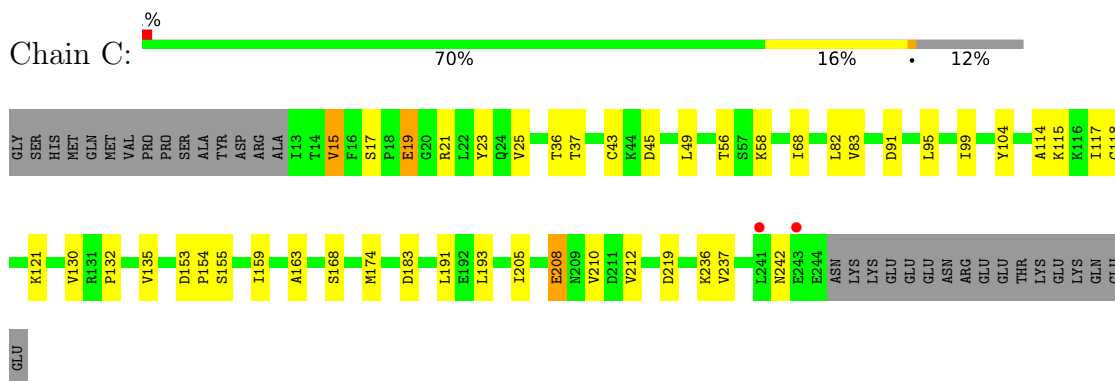
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

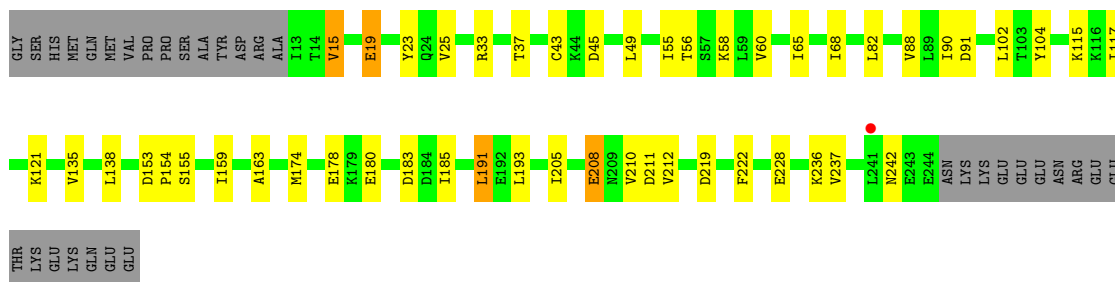


- Molecule 1: Proteasome subunit alpha



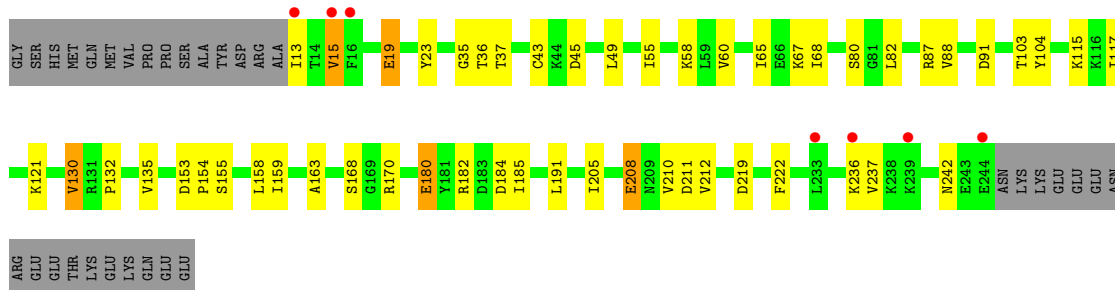
- Molecule 1: Proteasome subunit alpha

Chain D: 



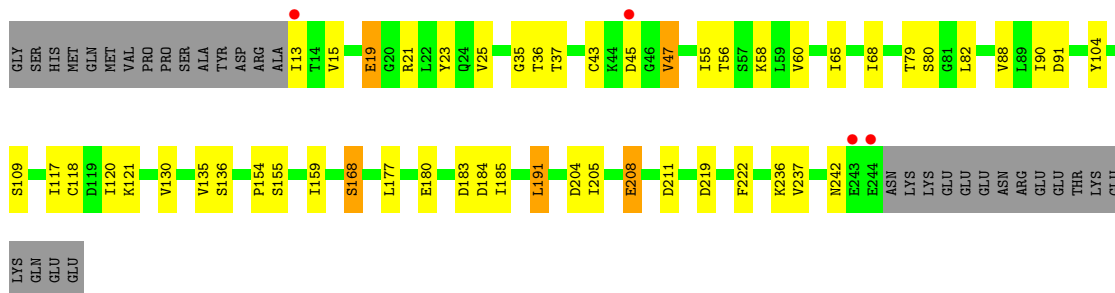
• Molecule 1: Proteasome subunit alpha

Chain E: 



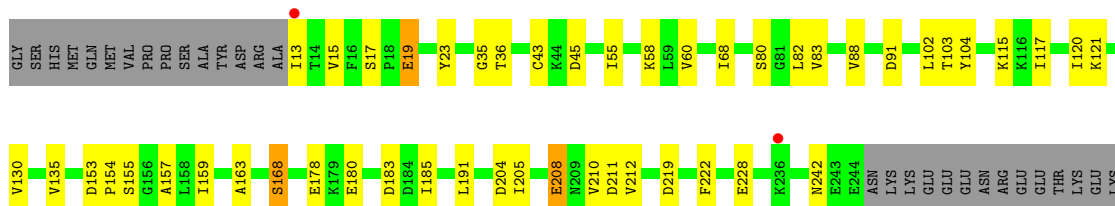
• Molecule 1: Proteasome subunit alpha

Chain F: 



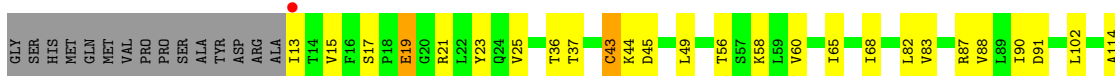
• Molecule 1: Proteasome subunit alpha

Chain G: 



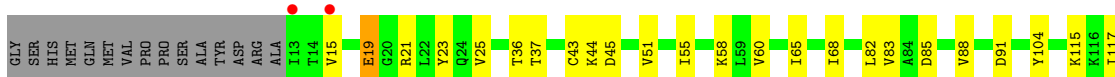
GLN
GLU
GLU

Molecule 1: Proteasome subunit alpha



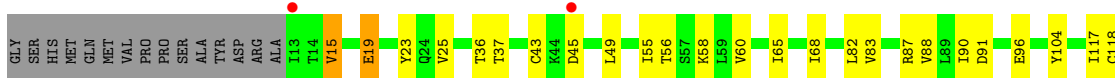
GLU
ASN
ARG
GLU
THR
LYS
GLU
LYS
GLN
GLU
GLU

Molecule 1: Proteasome subunit alpha



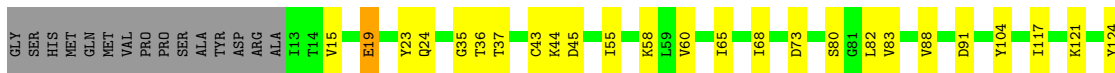
GLU
GLU
THR
LYS
GLU
LYS
GLN
GLU
GLU

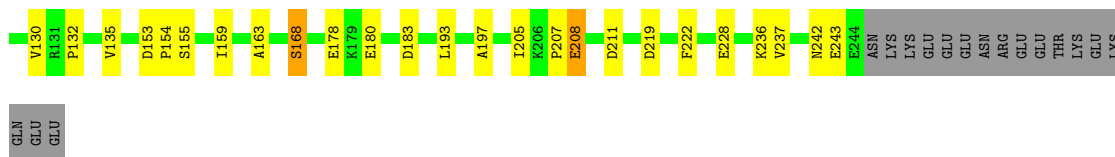
Molecule 1: Proteasome subunit alpha



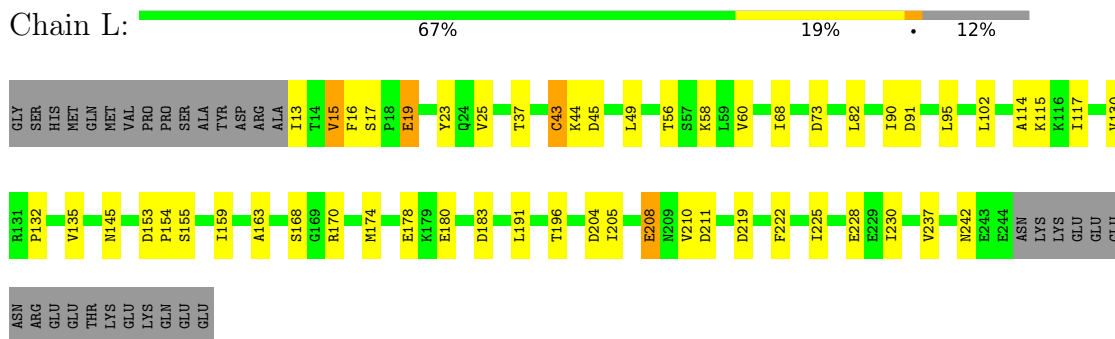
GLU

Molecule 1: Proteasome subunit alpha

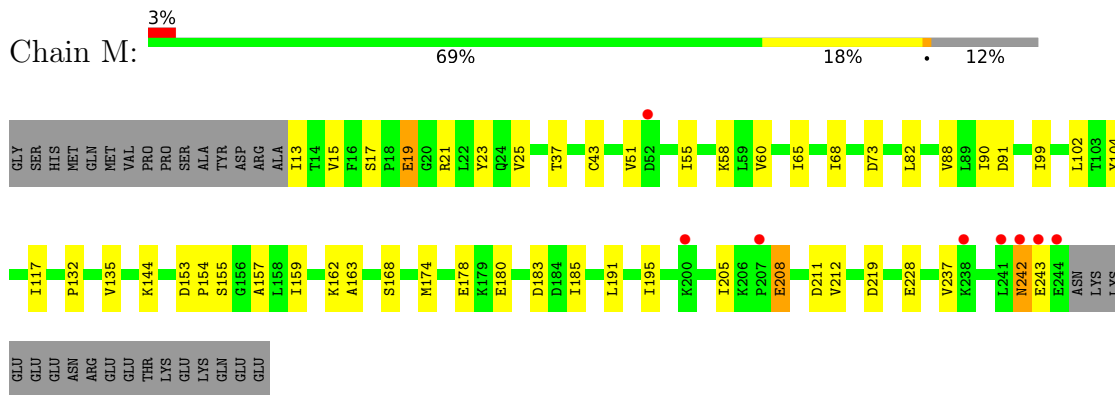




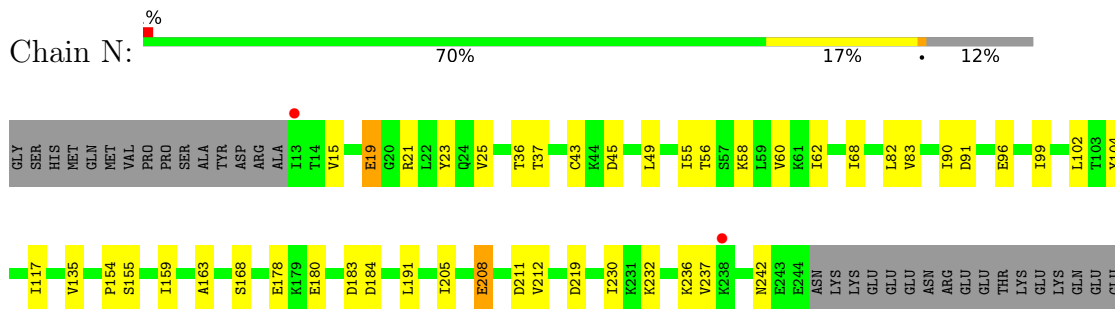
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha



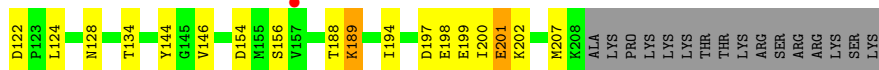
• Molecule 1: Proteasome subunit alpha



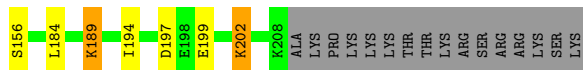
• Molecule 2: Proteasome subunit beta



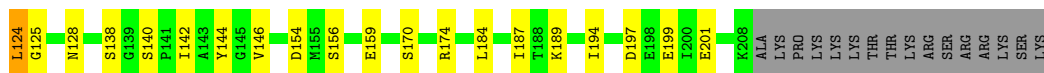
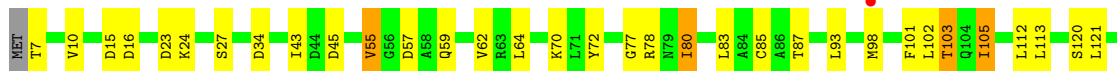
• Molecule 2: Proteasome subunit beta



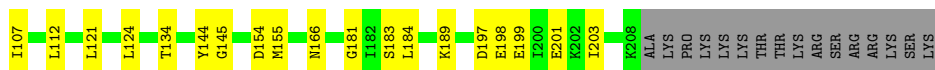
• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta

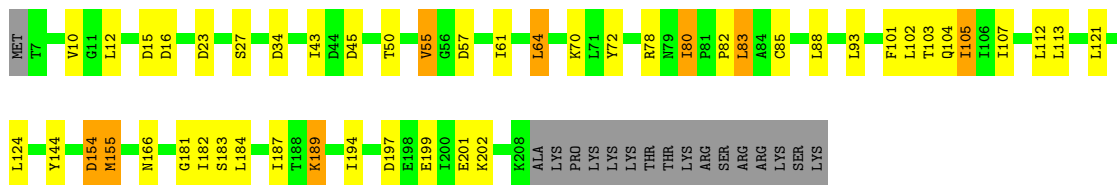


• Molecule 2: Proteasome subunit beta

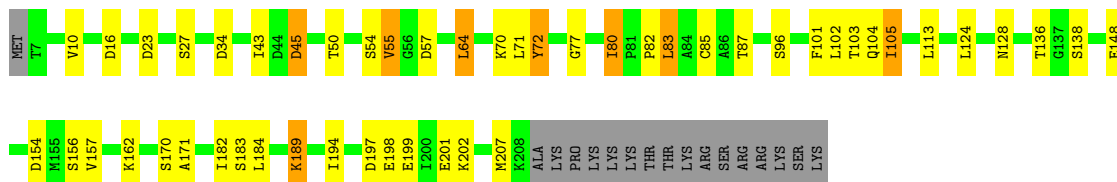


• Molecule 2: Proteasome subunit beta

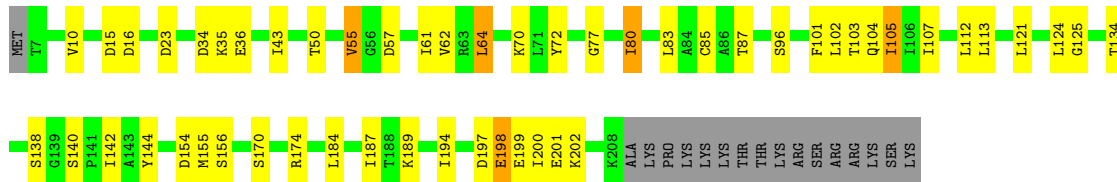




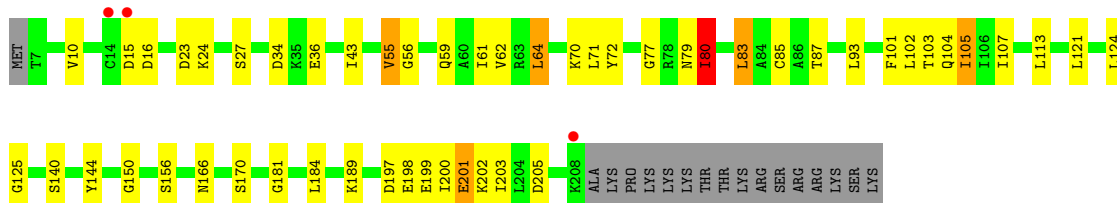
• Molecule 2: Proteasome subunit beta



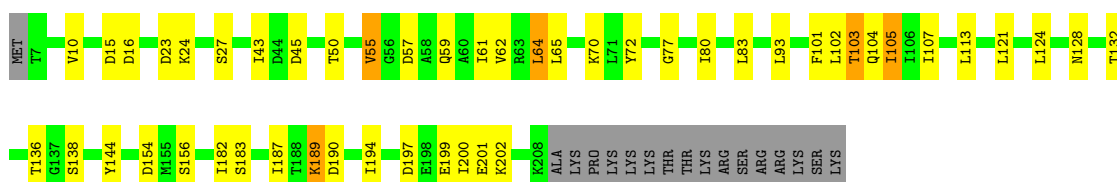
• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta

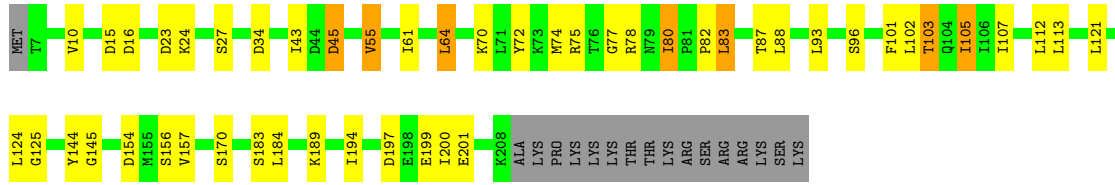


• Molecule 2: Proteasome subunit beta

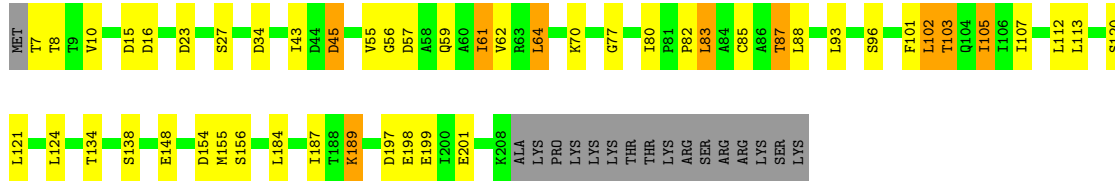


• Molecule 2: Proteasome subunit beta

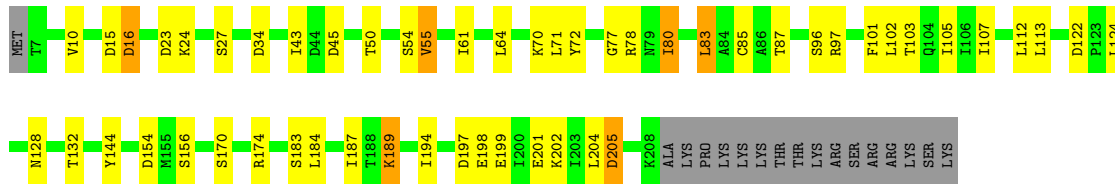




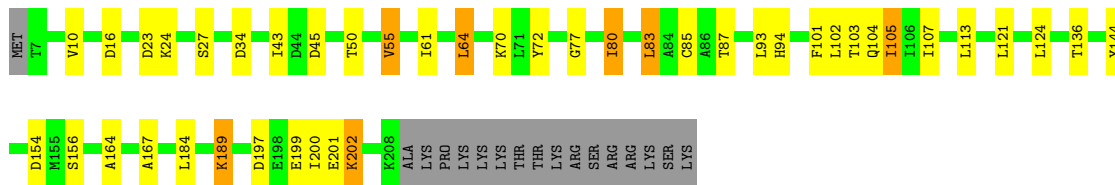
• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	206.72Å 219.54Å 149.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 4.10 49.98 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.98-4.10) 99.8 (49.98-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 4.14Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.254 , 0.325 0.243 , 0.310	Depositor DCC
R_{free} test set	2740 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	118.1	Xtrriage
Anisotropy	0.499	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 121.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	46648	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6646e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/1832	0.66	0/2468
1	B	0.47	0/1832	0.67	0/2468
1	C	0.50	0/1832	0.69	0/2468
1	D	0.57	1/1832 (0.1%)	0.76	2/2468 (0.1%)
1	E	0.48	0/1832	0.69	1/2468 (0.0%)
1	F	0.57	0/1832	0.72	1/2468 (0.0%)
1	G	0.55	0/1832	0.73	0/2468
1	H	0.50	0/1832	0.69	1/2468 (0.0%)
1	I	0.49	0/1832	0.70	1/2468 (0.0%)
1	J	0.53	0/1832	0.69	0/2468
1	K	0.51	0/1832	0.69	0/2468
1	L	0.53	0/1832	0.70	0/2468
1	M	0.48	0/1832	0.67	0/2468
1	N	0.47	0/1832	0.65	0/2468
2	a	0.52	0/1536	0.72	0/2070
2	b	0.52	0/1536	0.74	1/2070 (0.0%)
2	c	0.51	0/1536	0.74	2/2070 (0.1%)
2	d	0.53	0/1536	0.77	1/2070 (0.0%)
2	e	0.55	0/1536	0.77	4/2070 (0.2%)
2	f	0.60	0/1536	0.80	1/2070 (0.0%)
2	g	0.58	0/1536	0.79	1/2070 (0.0%)
2	h	0.53	0/1536	0.75	1/2070 (0.0%)
2	i	0.57	0/1536	0.79	2/2070 (0.1%)
2	j	0.61	0/1536	0.84	1/2070 (0.0%)
2	k	0.59	0/1536	0.79	1/2070 (0.0%)
2	l	0.54	0/1536	0.79	3/2070 (0.1%)
2	m	0.51	0/1536	0.75	1/2070 (0.0%)
2	n	0.50	0/1536	0.74	1/2070 (0.0%)
All	All	0.53	1/47152 (0.0%)	0.73	26/63532 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	91	ASP	CB-CG	5.38	1.63	1.51

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	i	64	LEU	CA-CB-CG	7.58	132.73	115.30
2	e	64	LEU	CA-CB-CG	7.57	132.70	115.30
2	d	64	LEU	CA-CB-CG	7.28	132.04	115.30
2	l	64	LEU	CA-CB-CG	6.86	131.09	115.30
2	n	64	LEU	CA-CB-CG	6.73	130.77	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/264 (87%)	163 (71%)	43 (19%)	24 (10%)	0	8
1	B	230/264 (87%)	162 (70%)	46 (20%)	22 (10%)	0	10
1	C	230/264 (87%)	155 (67%)	51 (22%)	24 (10%)	0	8
1	D	230/264 (87%)	158 (69%)	47 (20%)	25 (11%)	0	7
1	E	230/264 (87%)	158 (69%)	47 (20%)	25 (11%)	0	7
1	F	230/264 (87%)	152 (66%)	53 (23%)	25 (11%)	0	7
1	G	230/264 (87%)	156 (68%)	51 (22%)	23 (10%)	0	9
1	H	230/264 (87%)	153 (66%)	49 (21%)	28 (12%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	230/264 (87%)	159 (69%)	44 (19%)	27 (12%)	0	6
1	J	230/264 (87%)	161 (70%)	45 (20%)	24 (10%)	0	8
1	K	230/264 (87%)	151 (66%)	51 (22%)	28 (12%)	0	5
1	L	230/264 (87%)	162 (70%)	39 (17%)	29 (13%)	0	5
1	M	230/264 (87%)	159 (69%)	45 (20%)	26 (11%)	0	6
1	N	230/264 (87%)	159 (69%)	48 (21%)	23 (10%)	0	9
2	a	200/219 (91%)	135 (68%)	45 (22%)	20 (10%)	0	9
2	b	200/219 (91%)	129 (64%)	53 (26%)	18 (9%)	1	12
2	c	200/219 (91%)	140 (70%)	45 (22%)	15 (8%)	1	15
2	d	200/219 (91%)	132 (66%)	46 (23%)	22 (11%)	0	7
2	e	200/219 (91%)	136 (68%)	46 (23%)	18 (9%)	1	12
2	f	200/219 (91%)	142 (71%)	42 (21%)	16 (8%)	1	14
2	g	200/219 (91%)	132 (66%)	43 (22%)	25 (12%)	0	5
2	h	200/219 (91%)	136 (68%)	44 (22%)	20 (10%)	0	9
2	i	200/219 (91%)	130 (65%)	46 (23%)	24 (12%)	0	5
2	j	200/219 (91%)	145 (72%)	39 (20%)	16 (8%)	1	14
2	k	200/219 (91%)	126 (63%)	50 (25%)	24 (12%)	0	5
2	l	200/219 (91%)	143 (72%)	37 (18%)	20 (10%)	0	9
2	m	200/219 (91%)	139 (70%)	43 (22%)	18 (9%)	1	12
2	n	200/219 (91%)	136 (68%)	46 (23%)	18 (9%)	1	12
All	All	6020/6762 (89%)	4109 (68%)	1284 (21%)	627 (10%)	0	8

5 of 627 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	TYR
1	A	43	CYS
1	A	132	PRO
1	A	155	SER
1	A	168	SER

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/224 (87%)	171 (88%)	24 (12%)	4	22
1	B	195/224 (87%)	167 (86%)	28 (14%)	3	18
1	C	195/224 (87%)	170 (87%)	25 (13%)	4	21
1	D	195/224 (87%)	170 (87%)	25 (13%)	4	21
1	E	195/224 (87%)	166 (85%)	29 (15%)	3	17
1	F	195/224 (87%)	165 (85%)	30 (15%)	2	16
1	G	195/224 (87%)	166 (85%)	29 (15%)	3	17
1	H	195/224 (87%)	162 (83%)	33 (17%)	2	14
1	I	195/224 (87%)	166 (85%)	29 (15%)	3	17
1	J	195/224 (87%)	170 (87%)	25 (13%)	4	21
1	K	195/224 (87%)	170 (87%)	25 (13%)	4	21
1	L	195/224 (87%)	166 (85%)	29 (15%)	3	17
1	M	195/224 (87%)	169 (87%)	26 (13%)	4	21
1	N	195/224 (87%)	170 (87%)	25 (13%)	4	21
2	a	163/179 (91%)	135 (83%)	28 (17%)	2	12
2	b	163/179 (91%)	126 (77%)	37 (23%)	1	5
2	c	163/179 (91%)	133 (82%)	30 (18%)	1	10
2	d	163/179 (91%)	128 (78%)	35 (22%)	1	6
2	e	163/179 (91%)	129 (79%)	34 (21%)	1	6
2	f	163/179 (91%)	125 (77%)	38 (23%)	1	5
2	g	163/179 (91%)	131 (80%)	32 (20%)	1	8
2	h	163/179 (91%)	126 (77%)	37 (23%)	1	5
2	i	163/179 (91%)	132 (81%)	31 (19%)	1	9
2	j	163/179 (91%)	126 (77%)	37 (23%)	1	5
2	k	163/179 (91%)	132 (81%)	31 (19%)	1	9
2	l	163/179 (91%)	127 (78%)	36 (22%)	1	6
2	m	163/179 (91%)	124 (76%)	39 (24%)	0	5
2	n	163/179 (91%)	132 (81%)	31 (19%)	1	9
All	All	5012/5642 (89%)	4154 (83%)	858 (17%)	2	13

5 of 858 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	51	VAL
1	M	68	ILE
2	m	71	LEU
1	I	159	ILE
1	I	45	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	g	128	ASN
1	N	98	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	232/264 (87%)	-0.08	4 (1%) 70 60	127, 157, 221, 336	0
1	B	232/264 (87%)	0.02	3 (1%) 77 68	118, 151, 270, 519	0
1	C	232/264 (87%)	-0.25	2 (0%) 84 77	114, 132, 205, 333	0
1	D	232/264 (87%)	-0.39	1 (0%) 92 87	59, 134, 205, 245	0
1	E	232/264 (87%)	-0.14	7 (3%) 50 39	82, 139, 252, 355	0
1	F	232/264 (87%)	-0.18	4 (1%) 70 60	92, 116, 204, 346	0
1	G	232/264 (87%)	-0.32	2 (0%) 84 77	106, 128, 215, 284	0
1	H	232/264 (87%)	-0.30	1 (0%) 92 87	131, 148, 187, 271	0
1	I	232/264 (87%)	-0.23	4 (1%) 70 60	90, 136, 212, 299	0
1	J	232/264 (87%)	-0.02	9 (3%) 39 31	81, 141, 259, 366	0
1	K	232/264 (87%)	-0.28	0 100 100	112, 139, 220, 291	0
1	L	232/264 (87%)	-0.25	0 100 100	113, 135, 208, 253	0
1	M	232/264 (87%)	-0.02	8 (3%) 45 36	126, 143, 253, 507	0
1	N	232/264 (87%)	-0.15	2 (0%) 84 77	130, 147, 186, 303	0
2	a	202/219 (92%)	-0.41	1 (0%) 91 85	118, 138, 170, 185	0
2	b	202/219 (92%)	-0.14	4 (1%) 65 56	113, 131, 161, 180	0
2	c	202/219 (92%)	-0.36	0 100 100	101, 119, 195, 251	0
2	d	202/219 (92%)	-0.40	1 (0%) 91 85	107, 124, 162, 194	0
2	e	202/219 (92%)	-0.42	1 (0%) 91 85	93, 111, 159, 203	0
2	f	202/219 (92%)	-0.37	0 100 100	100, 115, 150, 175	0
2	g	202/219 (92%)	-0.33	0 100 100	110, 125, 149, 171	0
2	h	202/219 (92%)	-0.40	0 100 100	123, 139, 174, 186	0
2	i	202/219 (92%)	-0.36	3 (1%) 73 63	110, 123, 155, 170	0
2	j	202/219 (92%)	-0.48	0 100 100	72, 87, 159, 212	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	k	202/219 (92%)	-0.43	0 100 100	80, 102, 177, 209	0
2	l	202/219 (92%)	-0.41	0 100 100	104, 120, 160, 193	0
2	m	202/219 (92%)	-0.35	0 100 100	102, 122, 213, 254	0
2	n	202/219 (92%)	-0.26	0 100 100	122, 148, 181, 195	0
All	All	6076/6762 (89%)	-0.27	57 (0%) 84 77	59, 134, 207, 519	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	244	GLU	6.5
1	J	13	ILE	5.3
1	E	236	LYS	5.2
1	J	244	GLU	4.6
1	A	244	GLU	4.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.